

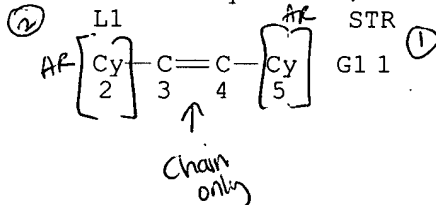
STRUCTURE FILE UPDATES: 8 MAY 2001 HIGHEST RN 334968-00-2
DICTIONARY FILE UPDATES: 3 MAY 2001 HIGHEST RN 334968-00-2

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

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① VAR G1=EU/TB/DY/SM/RU/OS
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
L3 19 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 11253 ITERATIONS
SEARCH TIME: 00.00.02

19 ANSWERS

L3 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 300542-94-3 REGISTRY

-----CN-----Ruthenium(1+), dichloro[2-(dicyclohexylphosphino-.kappa.P)-N,N,N-

trimethylethanaminium][[3-[2-[4-(methoxycarbonyl)phenyl]ethenyl]cyclopentylmethylene]- (9CI) (CA INDEX NAME)

MF C33 H53 Cl2 N O2 P Ru

CI CCS

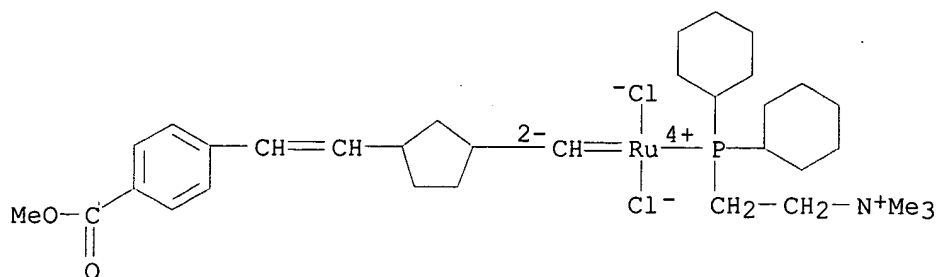
SR CA

LC STN Files: CA, CAPLUS

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MEC



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:281426 Mechanistic Studies of Olefin Metathesis by Ruthenium Carbene Complexes Using Electrospray Ionization Tandem Mass Spectrometry. Adlhart, Christian; Hinderling, Christian; Baumann, Harold;

Chen, Peter (Laboratorium fuer Organische Chemie, Eidgenoessischen Technischen Hochschule, Zurich, Switz.). J. Am. Chem. Soc., 122(34), 8204-8214 (English) 2000. CODEN: JACSAT. ISSN: 0002-7863. Publisher: American Chemical Society.

AB The olefin metathesis reaction of the Grubbs ruthenium carbene complexes has been investigated in the gas phase by electrospray ionization tandem mass spectrometry. Relative rates of reaction for substituted ruthenium benzylidenes and alkylidenes after removal of one phosphine ligand were interpreted with the aid of linear free energy anal. and kinetic isotope effects. The exptl. observations are consistent with a reaction profile in which the metallacyclobutane structure is a transition state rather than an intermediate, although alternative explanations cannot be wholly ruled out. Electron withdrawal on the carbene moiety is found to accelerate the metathesis reaction when only the metathesis step itself

is

examd. Quantum chem. calcns. at a variety of levels were performed to check for the consistency of the interpretation.

L3 ANSWER 2 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 270586-96-4 REGISTRY

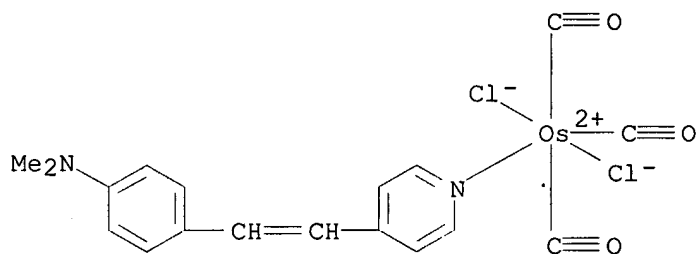
CN Osmium, tricarbonyldichloro[N,N-dimethyl-4-[(1E)-2-(4-pyridinyl-.kappa.N)ethenyl]benzenamine]-, (OC-6-33)- (9CI)' (CA INDEX NAME)

MF C18 H16 Cl2 N2 O3 Os

CI CCS

SR CA

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 133:4791 Quadratic Hyperpolarizability Enhancement of para-Substituted Pyridines upon Coordination to Organometallic Moieties: The Ambivalent Donor or Acceptor Role of the Metal. Roberto, Dominique; Ugo, Renato; Bruni, Silvia; Cariati, Elena; Cariati, Franco; Fantucci, PierCarlo; Invernizzi, Ivana; Quici, Silvio; Ledoux, Isabelle; Zyss, Joseph (Dipartimento di Chimica Inorganica Metallorganica e Analitica and Centro CNR CSSSCMTBSO, Universita di Milano, Milan, I-20133, Italy). Organometallics, 19(9), 1775-1788 (English) 2000. CODEN: ORGND7. ISSN: 0276-7333. Publisher: American Chemical Society.

AB Coordination of para-substituted pyridines 4-X-C₅H₄N (X = NMe₂, CMe₃, H, COMe, CN) to metal carbonyl moieties such as cis-M(CO)₂Cl (M = Rh(I), Ir(I)) and fac-Os(CO)₃Cl₂ produces an enhancement up to .apprx.2 orders

of magnitude of the quadratic hyperpolarizability .beta..lambda. of the free pyridine. This effect is due either to a red shift of the intraligand charge-transfer (ILCT) transition upon coordination (when X is a strong electron donor) or to a significant effect on the metal-to-ligand charge-transfer (MLCT) transitions (when X is a strong electron acceptor).

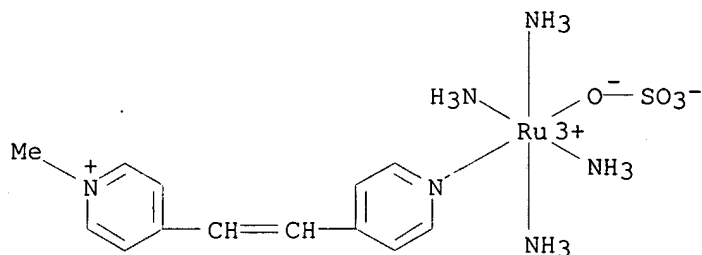
In this latter case the quadratic hyperpolarizability may assume a neg. sign, due to the neg. value of .DELTA..mu.eg upon excitation. Therefore as already shown by metal carbonyl moieties such as M(CO)₅ (M = Cr, W), a soft metal center displays, from the point of view of the perturbation of the quadratic hyperpolarizability of pyridines, an ambivalent acceptor or donor role. The quadratic hyperpolarizability of complexes of more .pi.-delocalized para-substituted pyridine ligands (X = trans- or trans,trans-(CH:CH)_nC₆H₄-4'-NMe₂ with n = 1 or 2) involving the same carbonyl Rh(I), Ir(I), and Os(II) moieties corresponds to an enhancement with respect to the free ligands of .apprx.1.5-2.3 times that when n = 1 and 1.5-1.7 times that when n = 2. This enhancement, which is relatively low when compared to simple pyridines, is dependent upon the length of

the .pi.-delocalized bridge (it decreases with increasing n) and upon the nature of the metal center (oxidn. state and ligand coordination sphere). Some of the complexes studied show significant values (between 400 .times.

10-30 and 600 .times. 10-30 D cm⁵ esu⁻¹) of the product .mu..beta.0.

L3 ANSWER 3 OF 19 REGISTRY COPYRIGHT 2001 ACS
RN 253781-14-5 REGISTRY

CN Ruthenium(2+), tetraammine[1-methyl-4-[2-(4-pyridinyl-.kappa.N)ethenyl]pyridinium][sulfato(2-)-.kappa.O]-, dichloride,
 (OC-6-23)- (9CI) (CA INDEX NAME)
 MF C13 H25 N6 O4 Ru S . 2 Cl
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



● 2 Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:87264 Tuning of charge-transfer absorption and molecular quadratic non-linear optical properties in ruthenium(II) ammine complexes.

Coe, Benjamin J.; Harris, James A.; Asselberghs, Inge; Persoons, Andre; Jeffery, John C.; Rees, Leigh H.; Gelbrich, Thomas; Hursthouse, Michael B.

(Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK). J. Chem. Soc., Dalton Trans. (20), 3617-3625 (English) 1999.

CODEN:

JCDTBI. ISSN: 0300-9246. Publisher: Royal Society of Chemistry.

AB The ligands N-methyl-2,7-diazapyrenium (Medap+), N-(2-pyrimidyl)-4,4'-bipyridinium (PymQ+), N-methyl-4-[trans-2-(4-pyridyl)ethenyl]pyridinium (Mebpe+) and N-phenyl-4-[trans-2-(4-pyridyl)ethenyl]pyridinium (Phbpe+) were used to prep. complex salts trans-[RuII(NH3)4(LD)(LA)][PF6]3 [LD = NH3 and LA = Medap+ 1, PymQ+ 2, Mebpe+ 3 or Phbpe+ 4; LD = pyridine (py) and LA = Medap+ 8, PymQ+ 9, Mebpe+ 10 or Phbpe+ 11; LD =

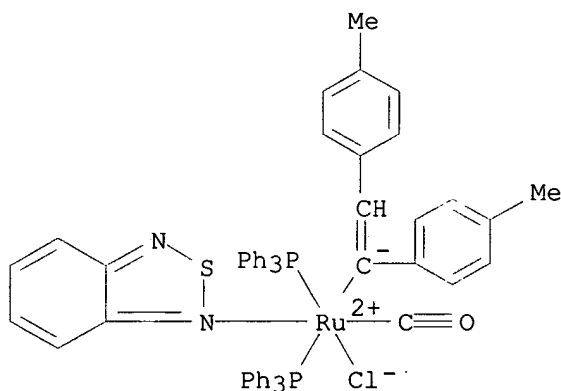
1-methylimidazole

(mim) and LA = Medap+ 12, PymQ+ 13, Mebpe+ 14 or Phbpe+ 15].

Trans-[RuII(NH3)4(py)(4,4'-bpy)][PF6]2 (4,4'-bpy = 4,4'-bipyridine) (16) also was prepd. The dipolar complexes in 1-4 and 8-15 exhibit intense d.p.i.(RuII).pi.*(LA) metal-to-ligand charge-transfer (MLCT) absorptions in the region 560-700 nm. For a given LA, the MLCT energy decreases as the donor strength of LD increases, in the order py < NH3 < mim. Within the pairs of Medap+/PymQ+ complexes, the energy of the Ru-based HOMO is const. and the MLCT energy decreases by .apprx.0.3 eV as the acceptor strength of LA increases on going from Medap+ to PymQ+. The complexes of Mebpe+ or Phbpe+ also have similar HOMO energies which are

lower than those of their Medap+/PymQ+ counterparts due to the increased basicity of LA. Replacement of Mebpe+ by Phbpe+ decreases the MLCT energy by .apprx.0.1 eV due to the greater electron-withdrawing ability of Phbpe+. Single-crystal structures of 8.cntdot.4MeCN and 16.cntdot.2MeCN were detd. Mol. 1st hyperpolarizabilities .beta. of 1-4 and 8-15, obtained from hyper-Rayleigh scattering measurements at 1064 nm, are in the range (579-1068) .times. 10-30 esu. Static hyperpolarizabilities .beta.0 derived by using the two-level model are also very large, with 13 having the largest at 336 .times. 10-30 esu. In general, .beta.0 increases as the absorption energy decreases, in keeping with the two-level model.

L3 ANSWER 4 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 213336-44-8 REGISTRY
 CN Ruthenium, (2,1,3-benzothiadiazole-.kappa.N1)[(1E)-1,2-bis(4-methylphenyl)ethenyl]carbonylchlorobis(triphenylphosphine)-, (OC-6-42)-(9CI) (CA INDEX NAME)
 MF C59 H49 Cl N2 O P2 Ru S
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



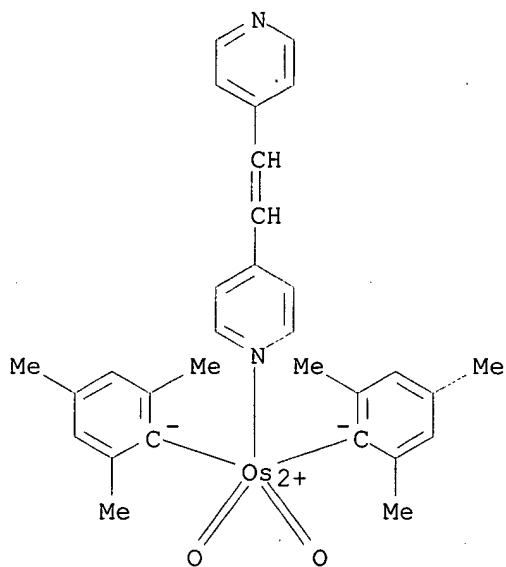
1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:245281 Polyazolyl Chelate Chemistry. 8. Organometallic Dihydridobis(pyrazol-1-yl)borato Complexes of Ruthenium(II). Hill, Anthony F.; White, Andrew J. P.; Williams, David J.; Wilton-Ely, James D. E. T. (Centre for Chemical Synthesis Department of Chemistry, Imperial College of Science Technology and Medicine, London, SW7 2AY, UK). Organometallics, 17(19), 4249-4258 (English) 1998. CODEN: ORGND7. ISSN: 0276-7333. Publisher: American Chemical Society.

AB Treatment of either [RuHCl(CO)(PPh3)3] or [RuH(CO)(NCMe)2(PPh3)2]BF4 with K[H2B(pz)2] (pz = pyrazol-1-yl) provides [RuH(CO)(PPh3)2{H2B(pz)2}] (1), which is also the product of the reaction of [Ru(SnPh3)Cl(CO)(PPh3)2] or [Ru(SiMe3)Cl(CO)(PPh3)2] with K[H2B(pz)2] in the presence of EtOH. [RuHCl(CS)(BTD)(PPh3)2] (BTD = 2,1,3-benzothiadiazole) and [RuHCl(CS)(BSD)(PPh3)2] (BSD = 2,1,3-benzoselenadiazole) were obtained

from the reactions of $[\text{RuHCl}(\text{CS})(\text{PPh}_3)_3]$ and BTD or BSD.
 $[\text{RuH}(\text{CS})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (2) was obtained in a manner similar to that for 1 from either $[\text{RuHCl}(\text{CS})(\text{PPh}_3)_3]$ or $[\text{RuHCl}(\text{CS})(\text{BTD})(\text{PPh}_3)_2]$ and $\text{K}[\text{H}_2\text{B}(\text{pz})_2]$. The σ -aryl complexes $[\text{RuPh}(\text{CA})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (A = O (3), S (4)) result from the reactions of $[\text{RuPhCl}(\text{CA})(\text{PPh}_3)_2]$ with $\text{K}[\text{H}_2\text{B}(\text{pz})_2]$. The σ -vinyl complexes
 $[\text{Ru}(\text{CR1:CHR2})\text{Cl}(\text{CO})(\text{BTD})(\text{PPh}_3)_2]$
(R1 = R2 = H (5), C6H4Me-4 (6); R1 = H, R2 = C6H4Me-4 (7), CPh2OH) react with $\text{K}[\text{H}_2\text{B}(\text{pz})_2]$ to provide $[\text{Ru}(\text{CR1:CHR2})(\text{CO})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (R1 = R2 = C6H4Me-4 (8); R1 = H, R2 = C6H4Me-4 (9), H (10), CPh2OH (11)). Treating $[\text{Ru}(\text{CPh:CHPh})\text{Cl}(\text{CS})(\text{PPh}_3)_2]$ with $\text{K}[\text{H}_2\text{B}(\text{pz})_2]$ provides $[\text{Ru}(\text{CPh:CHPh})(\text{CS})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (13), which reacts rapidly with CO to give the thioacyl complex $[\text{Ru}(\eta^2\text{-SCCPh:CHPh})(\text{CO})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (14) by loss of phosphine. The alkynyl derivs.
 $[\text{Ru}(\text{C.tplbond.CR})(\text{CO})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (R = C6H4Me-4 (15), CPh2OH (16)) were prep'd. from the reaction of
 $[\text{Ru}(\text{CH:CHC}_6\text{H}_4\text{Me-4})(\text{CO})(\text{PPh}_3)_2\{\text{H}_2\text{B}(\text{pz})_2\}]$ (9) with excess HC.tplbond.CR or alternatively from the reaction of 1 with $[\text{Hg}(\text{C.tplbond.CC}_6\text{H}_4\text{Me-4})_2]$.
The crystal structure of 10 is also reported.

L3 ANSWER 5 OF 19 REGISTRY COPYRIGHT 2001 ACS
RN 174646-11-8 REGISTRY
CN Osmium, [4,4'-(1,2-ethenediyl)bis[pyridine]-N]dioxobis(2,4,6-trimethylphenyl)-, (E)- (9CI) (CA INDEX NAME)
MF C30 H32 N2 O2 Os
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:232727 Reactions of Dimesityldioxoosmium(VI) with Bidentate

N-Heterocycles. Crystal Structure of a Dioxoosmium(VI) Complex Containing a Molecular Square. Leung, Wa-Hung; Cheng, Jack Y. K.; Hun, Tom S. M.; Che, Chi-Ming; Wong, Wing-Tak; Cheung, Kung-Kai (Department of Chemistry, Hong Kong University of Science and Technology, Kowloon, Hong Kong). Organometallics, 15(5), 1497-501 (English) 1996. CODEN: ORGND7. ISSN: 0276-7333.

AB The interaction of $\text{OsO}_2(\text{mes})_2$ (mes = mesityl) with pyz (pyrazine) gave the

pyrazine-bridged dimer $[\text{OsO}_2(\text{mes})_2]_2(\mu\text{-pyz})$ (1), which was characterized by x-ray crystallog. The structure around Os in 1 is square

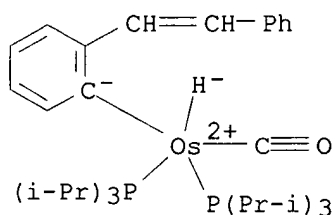
pyramidal, with the pyrazine, two oxo ligands, and one mesityl group in the square plane. The Os-O distance and O-Os-O angle are 1.71 Å and 147.5°, resp. The reaction of $\text{OsO}_2(\text{mes})_2$ with 4,4'-bpy (4,4'-bipyridyl) and bpe (trans-1,2-bis(4-pyridyl)ethylene) in Et₂O gave the oligomeric $[\text{OsO}_2(\text{mes})_2\text{L}]_n$ (L = 4,4'-bpy (2), bpe (3)) in good yields. The ¹H-NMR spectra of 2 and 3 indicate that L's are coordinated in a sym. fashion in these oligomers. The reaction of $\text{OsO}_2(\text{mes})_2$ with 4,4'-bpy in CHCl₃ followed by slow evapn. afforded the cryst. tetramer $[\text{OsO}_2(\text{mes})_2(\mu\text{-4,4'-bpy})]_4$ (4). The crystal structure of the tetramer

4 contains the square-planar $[\text{Os}(4,4'\text{-bpy})]_4$ core with octahedral local geometry around each Os. The Os-O distance and O-Os-O angle are 1.6 Å and 159°, resp.

Treatment of $\text{OsO}_2(\text{mes})_2$ with CNpy (4-cyanopyridine) gave $[\text{OsO}_2(\text{mes})_2]_2 \cdot [\text{OsO}_2(\text{mes})_2(\text{CNpy})]$ (5). The structure of 5 consists of the four-coordinate $[\text{OsO}_2(\text{mes})_2]$ and

five-coordinate $[\text{OsO}_2(\text{mes})_2(\text{CNpy})]$ moieties, which are linked together via the $\text{Os}:\text{O}\cdots\cdots\cdots\text{Os}$ interaction. The Os-O distances in the $[\text{OsO}_2(\text{mes})_2]$ and $[\text{OsO}_2(\text{mes})_2(\text{CNpy})]$ moieties in 5 are 1.69 and 1.71 .ANG., resp. The $(\text{Os})\text{O}\cdots\cdots\cdots\text{Os}$ distance is 2.78 .ANG., and the Os-O $\cdots\cdots\cdots\text{Os}$ angle is 170.degree.. The Os-O stretching frequency for the above dimesityldioxoosmium(VI) complexes correlates well with the Os-O bond order and the coordination environment around Os.

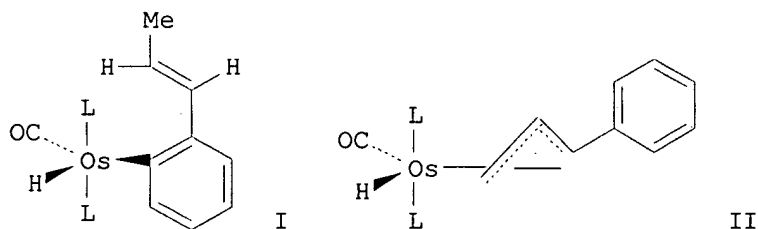
L3 ANSWER 6 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 173378-46-6 REGISTRY
 CN Osmium, carbonylhydro[2-(2-phenylethenyl)phenyl]bis[tris(1-methylethyl)phosphine]-, [SP-5-41-(E)]- (9CI) (CA INDEX NAME)
 MF C33 H54 O Os P2
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

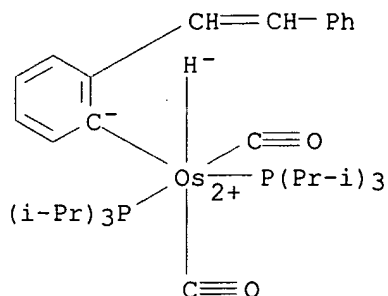
REFERENCE 1: 124:146440 Carbon-Carbon Coupling and Carbon-Hydrogen Activation Reactions in Bis(triisopropylphosphine)osmium Complexes. Esteruelas, Miguel A.; Lahoz, Fernando J.; Onate, Enrique; Oro, Luis A.; Sola, Eduardo (Instituto de Ciencia de Materiales de Aragon;, Universidad de Zaragoza, Zaragoza, 50009, Spain). J. Am. Chem. Soc., 118(1), 89-99 (English) 1996. CODEN: JACSAT. ISSN: 0002-7863.

GI



AB Reaction of the alkenyl complex $\text{OsCl}(\text{E-CH:CHPh})(\text{CO})(\text{PiPr}_3)_2$ (1) with phenyllithium gives $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHPh)}\}(\text{CO})(\text{PiPr}_3)_2$ (2). The structure of 2 (isomer 2a) was detd. by x-ray diffraction: triclinic, space group P.hivin.1; a 9.230(1), b 10.092(1), c 18.525(2) .ANG., .alpha. 88.667(7), .beta. 87.172(7), .gamma. 71.110(6).degree., Z = 2, R (F, Fo .gtoreq. 4.sigma.(Fo)) = 4.01, wR (F2, all reflections) = 9.94%. The geometry around the Os can be described as a distorted octahedron with the two triisopropylphosphine ligands occupying two relative trans positions. The remaining perpendicular plane is formed by the carbonyl and the 2-(E-1'-styryl)phenyl ligands mutually trans disposed, the hydride ligand and one olefinic H of the 2-(E-1'-styryl)phenyl ligand, which shows an agostic interaction with the Os atom (distance 2.05(7) .ANG.). The solns. of 2 show equil. between the agostic isomer (2a) and a nonagostic isomer (2b). The thermodyn. magnitudes involved in the equil. as well as the activation parameters for the conversion between the two isomers were detd. in toluene-d8 by 1H NMR spectroscopy. The values obtained were .DELTA.H.degree. = -1.6 (.-.0.1) Kcal mol-1 and .DELTA.S.degree. = -9.6 (.-.0.6) cal K-1 mol-1 for the formation of the agostic isomer, whereas the activation parameters for the breaking of the agostic interaction were .DELTA.H.thermod. = 7.6 (.-.0.2) Kcal mol-1 and .DELTA.S.thermod. = -1.0 (.-.0.7) cal K-1 mol-1. 2 Reacts with CO to give the octahedral complex $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHPh)}\}(\text{CO})_2(\text{PiPr}_3)_2$ (3). Reactions of 1 with methylolithium and CD_3Li give $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHCH}_3)\}(\text{CO})(\text{PiPr}_3)_2$ (4; shown as I (L = PiPr3)) and $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHCD}_3)\}(\text{CO})(\text{PiPr}_3)_2$ (4-d3), resp. The spectra of these complexes indicate that in soln. they also show equil. between agostic and nonagostic isomers. Reactions of 4 with P(OMe)_3 and CO afford $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHCH}_3)\}(\text{CO})\{\text{P(OMe)}_3\}(\text{PiPr}_3)_2$ (5) and $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHCH}_3)\}(\text{CO})_2(\text{PiPr}_3)_2$ (6), resp., in which the incoming ligands coordinate trans to the hydride. 4 And 4-d3 isomerize in soln. to give $\text{OsH}(\text{.eta.3-CH}_2\text{CHCHPh})(\text{CO})(\text{PiPr}_3)_2$ (11; shown as II (L = PiPr3)) and $\text{OsD}(\text{.eta.3-CD}_2\text{CHCHPh})(\text{CO})(\text{PiPr}_3)_2$ (11-d3), resp. Reaction of 11 with CO leads to $\text{OsH}(\text{.eta.1-CH}_2\text{CH:CHPh})(\text{CO})_2(\text{PiPr}_3)_2$ (12). The 1st order consts. kobs and kobs-d3 for the isomerization of 4 and 4-d3 to 11 and 11-d3 were obtained in CDCl_3 , giving activation parameters of .DELTA.H.thermod. = 20.8 (.-.1.7) Kcal mol-1 and .DELTA.S.thermod. = -2.8 (.-.2.0) cal K-1 mol-1 for the isomerization of 4 to 11 and a relation kobs/kobs-d3 = 3.6 at 303 K.

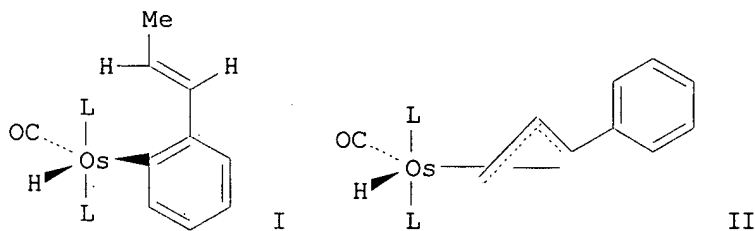
L3 ANSWER 7 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 173378-40-0 REGISTRY
 CN Osmium, dicarbonylhydro[2-(2-phenylethenyl)phenyl]bis[tris(1-methylethyl)phosphine]-, [OC-6-14-(E)]- (9CI) (CA INDEX NAME)
 MF C34 H54 O2 Os P2
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 124:146440 Carbon-Carbon Coupling and Carbon-Hydrogen Activation Reactions in Bis(triisopropylphosphine)osmium Complexes. Esteruelas, Miguel A.; Lahoz, Fernando J.; Onate, Enrique; Oro, Luis A.; Sola, Eduardo (Instituto de Ciencia de Materiales de Aragon, Universidad de Zaragoza, Zaragoza, 50009, Spain). J. Am. Chem. Soc., 118(1), 89-99 (English) 1996. CODEN: JACSAT. ISSN: 0002-7863.

GI



AB Reaction of the alkenyl complex $\text{OsCl}(\text{E-CH:CHPh})(\text{CO})(\text{PiPr}_3)_2$ (1) with phenyllithium gives $\text{OsH}\{\text{C}_6\text{H}_4\text{-2-(E-CH:CHPh)}\}(\text{CO})(\text{PiPr}_3)_2$ (2). The structure of 2 (isomer 2a) was detd. by x-ray diffraction: triclinic, space group P.hivin.1, a 9.230(1), b 10.092(1), c 18.525(2) .ANG., .alpha.

88.667(7), .beta. 87.172(7), .gamma. 71.110(6).degree., Z = 2, R (F, Fo .gtoreq. 4.sigma.(Fo)) = 4.01, wR (F2, all reflections) = 9.94%. The geometry around the Os can be described as a distorted octahedron with

the

two triisopropylphosphine ligands occupying two relative trans positions. The remaining perpendicular plane is formed by the carbonyl and the 2-(E-1'-styryl)phenyl ligands mutually trans disposed, the hydride ligand and one olefinic H of the 2-(E-1'-styryl)phenyl ligand, which shows an agostic interaction with the Os atom (distance 2.05(7) .ANG.). The

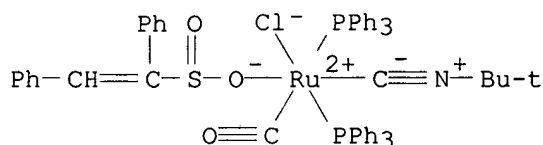
solns.

of 2 show equil. between the agostic isomer (2a) and a nonagostic isomer (2b). The thermodyn. magnitudes involved in the equil. as well as the activation parameters for the conversion between the two isomers were detd. in toluene-d8 by 1H NMR spectroscopy. The values obtained were

.DELTA.H.degree. = -1.6 (±.0.1) Kcal mol⁻¹ and .DELTA.S.degree. = -9.6 (±.0.6) cal K⁻¹ mol⁻¹ for the formation of the agostic isomer, whereas the activation parameters for the breaking of the agostic interaction were

.DELTA.H.thermod. = 7.6 (±.0.2) Kcal mol⁻¹ and .DELTA.S.thermod. = -1.0 (±.0.7) cal K⁻¹ mol⁻¹. 2 Reacts with CO to give the octahedral complex OsH{C₆H₄-2-(E-CH:CHPh)}(CO)₂(PiPr₃)₂ (3). Reactions of 1 with methylolithium and CD₃Li give OsH{C₆H₄-2-(E-CH:CHCH₃)}(CO)(PiPr₃)₂ (4; shown as I (L = PiPr₃)) and OsH{C₆H₄-2-(E-CH:CHCD₃)}(CO)(PiPr₃)₂ (4-d₃), resp. The spectra of these complexes indicate that in soln. they also show equil. between agostic and nonagostic isomers. Reactions of 4 with P(OMe)₃ and CO afford OsH{C₆H₄-2-(E-CH:CHCH₃)}(CO){P(OMe)₃}(PiPr₃)₂ (5) and OsH{C₆H₄-2-(E-CH:CHCH₃)}(CO)₂(PiPr₃)₂ (6), resp., in which the incoming ligands coordinate trans to the hydride. 4 And 4-d₃ isomerize in soln. to give OsH(.eta.³-CH₂CHCHPh)(CO)(PiPr₃)₂ (11; shown as II (L = PiPr₃)) and OsD(.eta.³-CD₂CHCHPh)(CO)(PiPr₃)₂ (11-d₃), resp. Reaction of 11 with CO leads to OsH(.eta.¹-CH₂CH:CHPh)(CO)₂(PiPr₃)₂ (12). The 1st order consts. k_{obs} and k_{obs}-d₃ for the isomerization of 4 and 4-d₃ to 11 and 11-d₃ were obtained in CDCl₃, giving activation parameters of .DELTA.H.thermod. = 20.8 (±.1.7) Kcal mol⁻¹ and .DELTA.S.thermod. = -2.8 (±.2.0) cal K⁻¹ mol⁻¹ for the isomerization of 4 to 11 and a relation k_{obs}/k_{obs}-d₃ = 3.6 at 303 K.

L3 ANSWER 8 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 163315-64-8 REGISTRY
 CN Ruthenium, carbonylchloro(2-isocyano-2-methylpropane)[.alpha.-(phenylmethylene)benzenemethanesulfinato-O]bis(triphenylphosphine)- (9CI)
 (CA INDEX NAME)
 MF C56 H50 Cl N O3 P2 Ru S
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



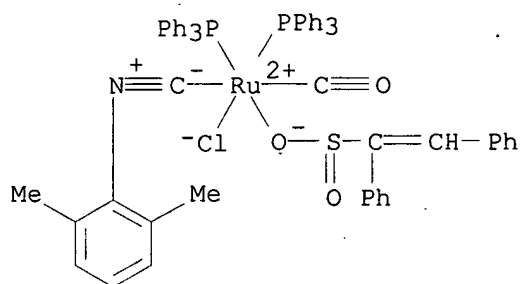
1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:305207 Hydrosulfination of alkynes: synthesis of vinyl sulfinato complexes of ruthenium(II). Hill, Anthony F. (Dep. Chem., Imperial Coll. Sci., London, SW7 2AY, UK). J. Chem. Soc., Chem. Commun. (7), 741-2 (English) 1995. CODEN: JCCCAT. ISSN: 0022-4936.

AB The reaction of [RuClH(CO)(PPh₃)₃] with alkynes (R1C.tplbond.CR2) and SO₂ provides the vinylsulfinato-S,O complexes [Ru(.eta.²-SO₂CR1:CHR2)Cl(CO)(PPh₃)₂] in a process reminiscent of hydroformylation.

L3 ANSWER 9 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 163315-58-0 REGISTRY
 CN Ruthenium, carbonylchloro(2-isocyano-1,3-dimethylbenzene)[.alpha.-(phenylmethylene)benzenemethanesulfinato-O]bis(triphenylphosphine)- (9CI)
 (CA INDEX NAME)
 MF C60 H50 Cl N O3 P2 Ru S
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS

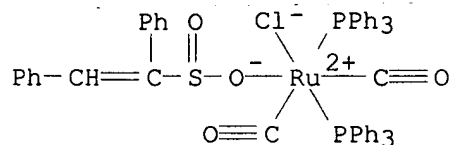


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:305207 Hydrosulfination of alkynes: synthesis of vinyl sulfinato complexes of ruthenium(II). Hill, Anthony F. (Dep. Chem., Imperial Coll. Sci., London, SW7 2AY, UK). J. Chem. Soc., Chem. Commun. (7), 741-2 (English) 1995. CODEN: JCCCAT. ISSN: 0022-4936.

AB The reaction of [RuClH(CO)(PPh3)3] with alkynes (R1C.tplbond.CR2) and SO2 provides the vinylsulfinate-S,O complexes [Ru(.eta.2-SO2CR1:CHR2)Cl(CO)(PPh3)2] in a process reminiscent of hydroformylation.

L3 ANSWER 10 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 163315-52-4 REGISTRY
 CN Ruthenium,
 dicarbonylchloro[.alpha.-(phenylmethylene)benzenemethanesulfina
 to-O]bis(triphenylphosphine)- (9CI) (CA INDEX NAME)
 MF C52 H41 Cl O4 P2 Ru S
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:305207 Hydrosulfination of alkynes: synthesis of vinyl

sulfinato complexes of ruthenium(II). Hill, Anthony F. (Dep. Chem., Imperial Coll. Sci., London, SW7 2AY, UK). J. Chem. Soc., Chem. Commun. (7), 741-2 (English) 1995. CODEN: JCCCAT. ISSN: 0022-4936.

AB The reaction of $[\text{RuClH}(\text{CO})(\text{PPh}_3)_3]$ with alkynes (R1C.tplbond.CR2) and SO_2 provides the vinylsulfinato-S,O complexes $[\text{Ru}(\eta^2\text{-SO}_2\text{CR1:CHR2})\text{Cl}(\text{CO})(\text{PPh}_3)_2]$ in a process reminiscent of hydroformylation.

L3 ANSWER 11 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 141054-08-2 REGISTRY

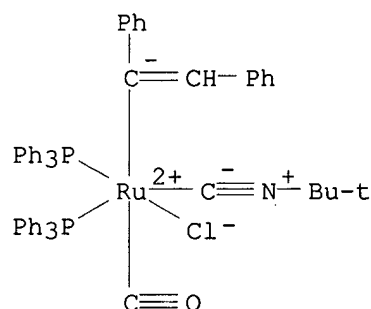
CN Ruthenium, carbonylchloro(1,2-diphenylethenyl)(2-isocyano-2-methylpropane)bis(triphenylphosphine)-, $[\text{OC-6-32-(E)}]^-$ (9CI) (CA INDEX NAME)

MF C56 H50 Cl N O P2 Ru

CI CCS

SR CA

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 116:214684 Reactions of alkenyl and alkynyl ruthenium(II) complexes with isocyanides: synthesis of .alpha.,.beta.-unsaturated .eta.1-acylruthenium(II) complexes and x-ray structure of

$[\text{Ru}(\text{C.tplbond.CPh})(\text{CNBu-tert})_3(\text{PPh}_3)_2]\text{PF}_6$. Montoya, Julio; Santos, Amelia; Lopez, Javier; Echavarren, Antonio M.; Ros, Josep; Romero, Antonio

(Inst. Cienc. Mater., CSIC, Madrid, 28006, Spain). J. Organomet. Chem., 426(3), 383-98 (English) 1992. CODEN: JORCAI. ISSN: 0022-328X.

AB Reaction of (E)-alkenyl complexes $\text{Ru}(\text{CO})\text{Cl}(\text{CH:CHR})(\text{PPh}_3)_2$ and $\text{Ru}(\text{CO})\text{Cl}(\text{CH:CHR})(\text{PPh}_3)_2\text{L}$ ($\text{R} = \text{Me}_3\text{C}$, Ph, etc.; $\text{L} = \text{Me}_2\text{Hpz}$, py) with an excess of an isocyanide $\text{R}'\text{NC}$ ($\text{R}' = \text{Me}_3\text{C}$, cyclohexyl) gives (E)-.alpha.,.beta.-unsatd.-.eta.1-acyl complexes

$[\text{Ru}(\text{COCH:CHR})(\text{CNR}')_3(\text{PPh}_3)_2]\text{Cl}$ in good yield. The corresponding reactions

with 1 equiv isocyanide give the hexacoordinate complexes $\text{Ru}(\text{CO})\text{Cl}(\text{CH:CHR})(\text{CNR}')(\text{PPh}_3)_2$. The reaction of $[\text{Ru}(\text{CO})(\text{CH:CHR})(\text{NCMe})_2(\text{PPh}_3)_2]\text{PF}_6$ with Me_3CNC also affords .eta.1-acyl complexes $[\text{Ru}(\text{COCH:CHR})(\text{CNCMe}_3)_3(\text{PPh}_3)_2]\text{PF}_6$. On the other hand,

treatment

of alkynyl complexes $[\text{Ru}(\text{CO})(\text{C.tplbond.CR})(\text{py})_2(\text{PPh}_3)_2]\text{PF}_6$ with an excess of Me_3CNC under forcing conditions promotes substitution of CO and

pyridine ligands by the isocyanide, yielding alkynyl derivs.
 $[\text{Ru}(\text{C.tplbond.CR})(\text{CNCMe}_3)_3(\text{PPh}_3)_2]\text{PF}_6$. An x-ray diffraction study of one of the complexes ($\text{R} = \text{Ph}$) confirmed the proposed structure. Similarly, reaction of the alkynyl complexes with CO gives only the ligand-substitution products $[\text{Ru}(\text{CO})_2(\text{C.tplbond.CR})(\text{py})(\text{PPh}_3)_2][\text{PF}_6]$.

L3 ANSWER 12 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 126206-47-1 REGISTRY

CN Ruthenium(1+),
 bis(acetonitrile)carbonyl(1,2-diphenylethenyl)bis(triphenyl
 phosphine)-, [OC-6-14-(E)]-, hexafluorophosphate(1-) (9CI) (CA INDEX
 NAME)

OTHER CA INDEX NAMES:

CN Benzene, 1,1'-(1,2-ethenediyl)bis-, ruthenium complex, (Z)-

MF C55 H47 N2 O P2 Ru . F6 P

SR CA

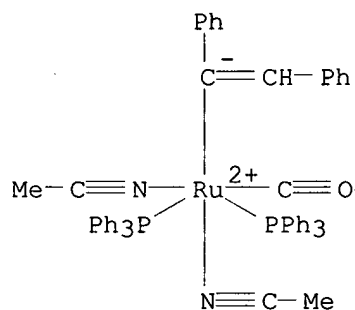
LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX, GMELIN*
 (*File contains numerically searchable property data)

CM 1

CRN 126206-46-0

CMF C55 H47 N2 O P2 Ru

CCI CCS

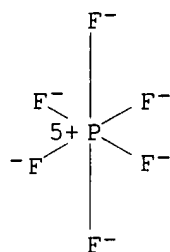


CM 2

CRN 16919-18-9

CMF F6 P

CGI CCS



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 115:182703 Phenylacetylene dimerization promoted by ruthenium(II) complexes. Echavarren, Antonio M.; Lopez, Javier; Santos, Amelia; Montoya, Julio (Inst. Quim. Org., CSIC, Madrid, 28006, Spain).

J. Organomet. Chem., 414(3), 393-400 (English) 1991. CODEN: JORCAI. ISSN: 0022-328X.

AB The complex $\text{Ru}(\text{CO})(\text{CH}:\text{CHPh})\text{Cl}(\text{C}_5\text{H}_5\text{N})(\text{PPh}_3)_2$ and related alkenyl complexes react in methanol or ethanol to give (E,E)-1,4-diphenylbuta-1,3-diene (I) and ruthenium(II) hydride $\text{Ru}(\text{CO})\text{H}(\text{Cl})(\text{C}_5\text{H}_5\text{N})(\text{PPh}_3)_3$. Further reaction of this hydride with the butadiene results in 1,2-redn. to yield (E)-1,4-diphenyl-1-butene. However, the reaction of phenylacetylene with catalytic amts. of ruthenium hydrides gave the dimer

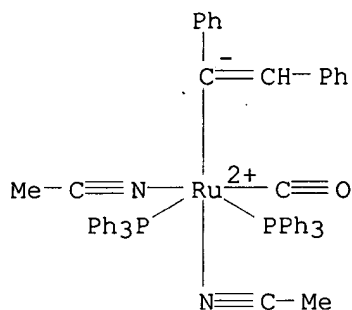
(Z)-1,4-diphenylbuten-3-yne. On the other hand, the reaction of 1,2-diphenylethenylruthenium(II) derivs. in methanol or ethanol gave trans-stilbene rather than the butadiene. Several deuteration expts. were

performed in order to elucidate the mechanism of formation of I and ruthenium hydride from the corresponding alkenyl complexes.

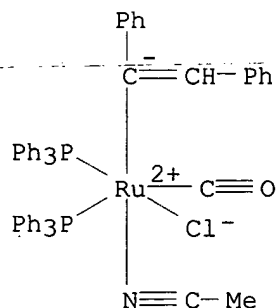
REFERENCE 2: 112:179398 Reactions of cationic ruthenium hydrido complexes $[\text{Ru}(\text{CO})\text{H}(\text{MeCN})_2(\text{PPh}_3)_2]\text{A}$ ($\text{A} = \text{ClO}_4, \text{PF}_6$) with alkynes. The crystal structure of $[\text{Ru}(\text{CO})(\text{MeOCC}:\text{CHCOOMe})(\text{MeCN})_2(\text{PPh}_3)_2]\text{ClO}_4$. Lopez, Javier; Romero, Antonio; Santos, Amelia; Vegas, Angel; Echavarren, Antonio M.; Noheda, Pedro (Inst. Cienc. Mater., CSIC, Madrid, 28006, Spain). J. Organomet. Chem., 373(2), 249-58 (English) 1989. CODEN: JORCAI. ISSN: 0022-328X.

AB Reactions of $[\text{Ru}(\text{CO})\text{H}(\text{MeCN})_2(\text{PPh}_3)_2]\text{X}$ with mono- and disubstituted acetylenes give the alkenyl derivs. $[\text{Ru}(\text{CO})(\text{RC}:\text{CHR}')(\text{MeCN})_2(\text{PPh}_3)_2]\text{X}$ ($\text{X} = \text{ClO}_4, \text{R} = \text{H}; \text{R}' = \text{Pr}, \text{CMe}_3, \text{Ph}, \text{CO}_2\text{Me}; \text{R} = \text{R}' = \text{CO}_2\text{Me}; \text{X} = \text{PF}_6, \text{R} = \text{R}' = \text{Ph}$) resulting from a cis-insertion of the alkyne into the Ru-H bond. The reaction of the perchlorate complex with diphenylacetylene yields alkenyl chlororuthenium derivs. resulting from the unexpected redn. of the perchlorate anion to chloride. The crystal structure of $[\text{Ru}(\text{CO})(\text{MeO}_2\text{CC}:\text{CHCO}_2\text{Me})(\text{MeCN})_2(\text{PPh}_3)_2]\text{ClO}_4$ has been detd. by x-ray crystallog. In this cationic complex both phosphine and acetonitrile mols. and, consequently, the carbonyl and alkenyl ligands are mutually trans, whereas in the other complexes only the phosphine ligands are in trans disposition, as inferred from ^1H NMR spectroscopic data.

L3 ANSWER 13 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 126206-46-0 REGISTRY
 CN Ruthenium(1+),
 bis(acetonitrile)carbonyl(1,2-diphenylethenyl)bis(triphenyl
 phosphine)-, [OC-6-14-(E)]- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Benzene, 1,1'-(1,2-ethenediyl)bis-, ruthenium complex, (Z)-
 MF C55 H47 N2 O P2 Ru
 CI CCS, COM
 SR CA
 LC STN Files: GMELIN*
 (*File contains numerically searchable property data)

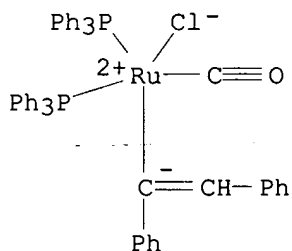


L3 ANSWER 14 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 126206-45-9 REGISTRY
 CN Ruthenium,
 (acetonitrile)carbonylchloro(1,2-diphenylethenyl)bis(triphenylp
 hosphine)-, [OC-6-52-(E)]- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Benzene, 1,1'-(1,2-ethenediyl)bis-, ruthenium complex, (Z)-
 MF C53 H44 Cl N O P2 Ru
 CI CCS
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, GMELIN*
 (*File contains numerically searchable property data)



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 112:179398 Reactions of cationic ruthenium hydrido complexes [Ru(CO)H(MeCN)2(PPh3)2]A (A = ClO4, PF6) with alkynes. The crystal structure of [Ru(CO)(MeOCC:CHCOOMe)(MeCN)2(PPh3)2]ClO4. Lopez, Javier; Romero, Antonio; Santos, Amelia; Vegas, Angel; Echavarren, Antonio M.; Noheda, Pedro (Inst. Cienc. Mater., CSIC, Madrid, 28006, Spain). J. Organomet. Chem., 373(2), 249-58 (English) 1989. CODEN: JORCAI. ISSN: 0022-328X.
- AB Reactions of [Ru(CO)H(MeCN)2(PPh3)2]X with mono- and disubstituted acetylenes give the alkenyl derivs. [Ru(CO)(RC:CHR')(MeCN)2(PPh3)2]X (X = ClO4, R = H; R' = Pr, CMe3, Ph, CO2Me; R = R' = CO2Me; X = PF6, R = R' = Ph) resulting from a cis-insertion of the alkyne into the Ru-H bond. The reaction of the perchlorate complex with diphenylacetylene yields alkenyl chlororuthenium derivs. resulting from the unexpected redn. of the perchlorate anion to chloride. The crystal structure of [Ru(CO)(MeO2CC:CHCO2Me)(MeCN)2(PPh3)2]ClO4 has been detd. by x-ray crystallog. In this cationic complex both phosphine and acetonitrile mols. and, consequently, the carbonyl and alkenyl ligands are mutually trans, whereas in the other complexes only the phosphine ligands are in trans disposition, as inferred from 1H NMR spectroscopic data.
- L3 ANSWER 15 OF 19 REGISTRY COPYRIGHT 2001 ACS
RN 109800-34-2 REGISTRY
CN Ruthenium,
carbonylchloro[(1E)-1,2-diphenylethenyl]bis(triphenylphosphine)-
, (TB-5-22)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, 1,1'-(1,2-ethenediyl)bis-, ruthenium complex, (Z)-
CN Ruthenium, carbonylchloro(1,2-diphenylethenyl)bis(triphenylphosphine)-,
[TB-5-22-(E)]-
MF C51 H41 Cl O P2 Ru
CI CCS
SR CA
LC STN Files: CA, CAPLUS, CASREACT, CHEMINFORMRX, GMELIN*
(*File contains numerically searchable property data)



16 REFERENCES IN FILE CA (1967 TO DATE)
16 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 132:293862 Mechanisms of C-Si and C-H Bond Formation on the Reactions of Alkenylruthenium(II) Complexes with Hydrosilanes. Maruyama,

Yooichiroh; Yamamura, Kunihiro; Sagawa, Takashi; Katayama, Hiroyuki; Ozawa, Fumiyuki (Department of Applied Chemistry Faculty of Engineering, Osaka City University, Sumiyoshi-ku Osaka, 558-8585, Japan). Organometallics, 19(7), 1308-1318 (English) 2000. CODEN: ORGND7. ISSN: 0276-7333. Publisher: American Chemical Society.

AB Reactions of the four alkenylruthenium(II) complexes $\text{Ru}[\text{C}(\text{R}_1):\text{CH}(\text{R}_2)]\text{Cl}(\text{CO})(\text{PPh}_3)_2$ ($\text{R}_1 = \text{H}$, $\text{R}_2 = \text{Ph}$ (1b); $\text{R}_1 = \text{H}$, $\text{R}_2 = t\text{-Bu}$ (1c); $\text{R}_1 = \text{Ph}$, $\text{R}_2 = \text{Ph}$ (1d); $\text{R}_1 = \text{CH}:\text{CH}(\text{SiMe}_3)$, $\text{R}_2 = \text{SiMe}_2\text{Ph}$ (1e)) with HSiMe_2Ph , which constitute the product-forming step of Ru-catalyzed hydrosilylation of alkynes, were examd. Two reaction courses are operative: one provides the C-Si coupling product $\text{PhMe}_2\text{SiC}(\text{R}_1):\text{CH}(\text{R}_2)$ and $\text{RuHCl}(\text{CO})(\text{PPh}_3)_3$ (path A), and the other forms the C-H coupling product $\text{HC}(\text{R}_1):\text{CH}(\text{R}_2)$ and $\text{Ru}(\text{SiMe}_2\text{Ph})\text{Cl}(\text{CO})(\text{PPh}_3)_2$ (path B). The ratio of the

two courses significantly varies with substituents on the alkenyl ligands, particularly with the α -substituent (R_1). Thus, 1b and 1c, without an α -substituent, react mainly by path A. In contrast, 1d and 1e, bearing an α -substituent, exclusively undergo path B. Kinetic studies using 1b and its para-substituted styryl ligand derivs. revealed that path A proceeds by direct interaction of the five-coordinated complexes with hydrosilane, without dissocn. of the PPh_3 ligand.

However, path B involves dissocn. of PPh_3 prior to the reaction of 1d or 1e with hydrosilane. Mechanisms of the C-Si and C-H bond formation are discussed with kinetic data.

REFERENCE 2: 129:330846 Synthesis and Reactivity of Ferrocenecarboxylate Ruthenium(II) Complexes. Catalytic Synthesis of a Ferrocenecarboxylic

Enol Ester. Matas, Lluïsa; Moldes, Isabel; Soler, Josep; Ros, Josep; Alvarez-Larena, Angel; Piniella, Joan F. (Departament de Química, Universitat Autònoma de Barcelona, Bellaterra, 08193, Spain). Organometallics, 17(21), 4551-4555 (English) 1998. CODEN: ORGND7. ISSN: 0276-7333. Publisher: American Chemical Society.

AB New ferrocenecarboxylate ruthenium(II) complexes were obtained from the reaction of $[\text{RuClH}(\text{CO})(\text{PPh}_3)_3]$ with ferrocenecarboxylic acid or its sodium

salt. The reaction of alkenyl complexes $[\text{Ru}(\text{O}_2\text{C}(\text{C}_5\text{H}_4)\text{Fe}(\text{C}_5\text{H}_5))(\text{CR}':\text{CRH})(\text{O})(\text{PPh}_3)_2]$ with CO and catalytic synthesis of the phenylethyleneferrocenecarboxylic ester have been studied. Thus, reaction of $[\text{RuClH}(\text{CO})(\text{PPh}_3)_3]$ with ferrocenecarboxylic acid gave $[\text{Ru}(\text{O}_2\text{C}(\text{C}_5\text{H}_4)\text{Fe}(\text{C}_5\text{H}_5))\text{Cl}(\text{CO})(\text{PPh}_3)_2]$ which was used as catalyst for addn. of ferrocenecarboxylic acid to phenylacetylene. The crystal structure of $[\text{Ru}(\text{O}_2\text{C}(\text{C}_5\text{H}_4)\text{Fe}(\text{C}_5\text{H}_5))(\text{CH}:\text{CH}_2)(\text{CO})(\text{PPh}_3)_2]$ was also detd.

REFERENCE 3: 129:302713 Reactions of alkenylruthenium(II) complexes with hydrosilane: C-Si vs. C-H bond formation. Maruyama, Yooichiroh;

Yamamura, Kunihiro; Ozawa, Fumiyuki (Department of Applied Chemistry, Faculty of Engineering, Osaka City University, Osaka, 558-8585, Japan). Chem. Lett. (9), 905-906 (English) 1998. CODEN: CMLTAG. ISSN: 0366-7022.

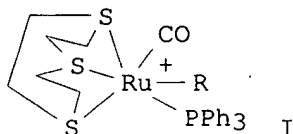
Publisher: Chemical Society of Japan.

AB Alkenylruthenium complexes, $\text{Ru}\{\text{C}(\text{R}1):\text{CH}(\text{R}2)\}\text{Cl}(\text{CO})(\text{PPh}_3)_2$ ($\text{R}1 = \text{H}$, $\text{R}2 = \text{Ph}$; $\text{R}1 = \text{H}$, $\text{R}2 = t\text{-Bu}$; $\text{R}1 = \text{Ph}$, $\text{R}2 = \text{Ph}$; $\text{R}1 = \text{CH}:\text{CH}(\text{SiMe}_3)$, $\text{R}2 = \text{SiMe}_2\text{Ph}$),

react with HSiMe_2Ph via two reaction courses (path A and path B), leading to C-Si and C-H bond formation, resp. Relative ratio of the two courses is strongly dependent upon steric bulkiness of substituent(s) on the alkenyl ligands. Reaction path A yields $(\text{Ph}_3\text{P})_3\text{Ru}(\text{CO})\text{Cl}(\text{H})$ and $\text{PhMe}_2\text{SiCR}1:\text{CHR}2$ in the presence of PPh_3 , whereas reaction path B yields $(\text{Ph}_3\text{P})_2\text{Ru}(\text{CO})\text{Cl}(\text{SiMe}_2\text{Ph})$ and $\text{R}1\text{CH}:\text{CHR}2$.

REFERENCE 4: 125:329020 Organometallic Macrocyclic Chemistry. 5. .sigma.-Vinyl and .sigma.-Aryl Complexes of Ruthenium(II) Ligated by 1,4,7-Trithiacyclononane: x-ray Crystal Structure of $[\text{Ru}(\text{CH}:\text{CH}_2)(\text{CO})(\text{PPh}_3)([\text{9}]_{\text{aneS}3})]\text{PF}_6 \cdot 2\text{CH}_2\text{Cl}_2$. Cannadine, Jason C.; Hill, Anthony F.; White, Andrew J. P.; Williams, David J.; Wilton-Ely, James D. E. T. (Department of Chemistry, Imperial College of Science Technology and Medicine, London, UK). Organometallics, 15(25), 5409-5415 (English) 1996. CODEN: ORGND7. ISSN: 0276-7333.

GI



AB The reaction of coordinatively unsatd. .sigma.-vinyl complexes $[\text{Ru}(\text{CR}:\text{CHR}')\text{Cl}(\text{CO})(\text{PPh}_3)_2]$ with 1,4,7-trithiacyclononane ($[\text{9}]_{\text{aneS}3}$) provides chiral salts of the half-sandwich complexes $[\text{Ru}(\text{CR}:\text{CHR}')(\text{CO})(\text{PPh}_3)([\text{9}]_{\text{aneS}3})]^+$, I ($\text{R} = \text{CH}:\text{CH}_2$, $\text{CPh}:\text{CHPh}$, $\text{CH}:\text{CHC}_6\text{H}_4\text{Me}-4$, $\text{C}(\text{C.tplbond.CPh}):\text{CHPh}$). The synthesis of the .sigma.-aryl complex $[\text{Ru}(\text{C}_6\text{H}_4\text{Me}-4)(\text{CO})(\text{PPh}_3)([\text{9}]_{\text{aneS}3})]^+$ is also described. A representative NMR study of one example allowed the assignment of individual chem. shifts for the 12 diastereotopic proton environments of the macrocycle. The crystal structure of $[\text{Ru}(\text{CH}:\text{CH}_2)(\text{CO})(\text{PPh}_3)([\text{9}]_{\text{aneS}3})]\text{PF}_6 \cdot 2\text{CH}_2\text{Cl}_2$ is also reported.

REFERENCE 5: 119:271376 Octahedral ruthenium(II) alkenyl complexes containing N.intrsec.S coordinated heterocyclic ligands. Gopinathan, Sarada; Deshpande, Shilpa S.; Gopinathan, Changaramponnath (Inorg. Chem. Div., Natl. Chem. Lab., Pune, 411008, India). Transition Met. Chem. (London), 18(6), 585-7 (English) 1993. CODEN: TMCHDN. ISSN: 0340-4285.

AB Hexacoordinated ruthenium(II) alkenyl complexes of the type $\text{Ru}(\text{CO})(\text{CR}:\text{CHPh})(\text{N.intrsec.S})(\text{PPh}_3)_2$ have been prepd. from coordinately unsatd. .alpha.-vinyl complexes $[\text{Ru}(\text{CO})\text{Cl}(\text{CR}:\text{CHPh})(\text{PPh}_3)_2]$ ($\text{R} = \text{H}$ or Ph) and the sodio-deriv. of the N.intrsec.S contg. heterocyclic ligands $[\text{N.intrsec.S} = 3,4\text{-substituted } 1,2,4\text{-triazole-5-thione and } 5\text{-alkylthio-1,3,4-thiadiazole-2-thione}]$ in a $\text{CH}_2\text{Cl}_2/\text{MeOH}$ mixt. at ambient temp. The complexes were characterized by their elemental anal. IR, ^1H and ^{31}P NMR spectra. An octahedral structure with trans-phosphorus ligands has been assigned on the basis of the spectral data.

- REFERENCE 6: 116:235841 Synthesis and reactivity of hydrido, halo, and .sigma.-organyl ruthenatetraboranes: Crystal structure of [RuH(B3H8)(CO)(PPh3)2]. Burns, Ian D.; Hill, Anthony F.; Thompson, Andrew R.; Alcock, Nathaniel W.; Claire, Kanwaljit S. (Dep. Chem., Imp. Coll., London, SW7 2AY, UK). J. Organomet. Chem., 425(1-2), C8-C10 (English) 1992. CODEN: JORCAI. ISSN: 0022-328X.
- AB The reactions of [RuClR(CO)(PPh3)n] (n = 2, R = .sigma.-vinyl, .sigma.-aryl; n = 3, R = H) with NMe4[B3H8] provide the ruthenatetraboranes [RuR(B3H8)(CO)(PPh3)2]. The crystal structure was detd. for the compd. with R = H. The latter reacts with N-halo succinimides to give the halo derivs. [RuR(B3H8)(CO)(PPh3)2] (R = Cl, Br, iodo) and with Me3CNC in CH2Cl2 to give [RuClH(CNCMe3)2(PPh3)2]. Sodium dialkyldithiocarbamate displaces the B3H8 moiety from the halo derivs., with formation of [Ru(S2CNMe2)2(CO)(PPh3)].
- REFERENCE 7: 115:232467 Polyazolyl chelate chemistry. 3. (.sigma.-Organyl)[tris(pyrazol-1-yl)borato]ruthenium complexes. Alcock, Nathaniel W.; Hill, Anthony F.; Melling, Richard P. (Dep. Chem., Univ. Warwick, Coventry, CV4 7AL, UK). Organometallics, 10(11), 3898-903 (English) 1991. CODEN: ORGND7. ISSN: 0276-7333.
- AB The reactions of K[HB(pz)3] (pz = pyrazol-1-yl) with the coordinatively unsatd. .sigma.-vinyl complexes [Ru(CR:CHR)Cl(CO)(PPh3)2] (R = H, Me, Ph) proceed with loss of a chloride and a phosphine ligand to provide the compds. [Ru(CR:CHR)(CO)(PPh3){HB(pz)3}] in high yield. Similar treatment of the complex [Ru(C6H4Me-4)Cl(CO)(PPh2)2] leads to the related .sigma.-aryl derivs. [Ru(C6H4Me-4)(CO)(PPh3){HB(pz)3}]. The .alpha.-(phenylethynyl)-trans-.beta.-styryl complex [Ru{C(C.tplbond.CPh):CHPh}(CO)(PPh3){HB(pz)3}] is obtained in high yield via the successive treatment of [RuClH(CO)(PPh3)3] with 1,4-diphenyl-1,3-butadiyne and K[HB(pz)3]. The mol. structure of [Ru{C(C.tplbond.CPh):CHPh}(CO)(PPh3){HB(pz)3}], detd. by x-ray diffraction, can be described as pseudooctahedral with 2 enantiomeric forms in the same asym. unit. The vinyl ligand is almost coplanar with the carbonyl ligand aligned in such a way as to maximize .pi.-retrodonative interactions.
- REFERENCE 8: 115:183545 Reaction of alkenylruthenium(II) Ru(CO)Cl(RC:CHR')(PPh3)2 complexes with carbon monoxide. Formation of dicarbonyl complexes or .eta.2-acyl complexes depending on the R and R' groups. Loumrhari, Hassane; Ros, Josep; Rosario Torres, M.; Santos, Amelia; Echavarren, Antonio M. (Dep. Quim., Univ. Auton. Barcelona, Bellaterra, 08193, Spain). J. Organomet. Chem., 411(1-2), 255-61 (English) 1991. CODEN: JORCAI. ISSN: 0022-328X.
- AB Reaction of the coordinatively unsatd. alkenyl complexes Ru(CO)Cl(RC:CHR')(PPh3)2 with CO gives two types of compds., the dicarbonyl complexes Ru(CO)2Cl(RC:CHR')(PPh3)2 (R = H, R' = H, Ph, CMe3, SiMe3, CO2Me, CO2Et; R = R' = CO2Me) and the .eta.2-acyl complexes Ru(CO)Cl(.eta.2-O:CCR:CHR')(PPh3)2 (R = R' = Me, Et, Ph). The reaction of sodium propionate with Ru(CO)Cl(.eta.2-O:CCMe:CHMe)(PPh3)2 yields a new product contg. both .eta.2-alkeneacyl and .eta.2-propionate ligands. The structures of the new complexes were established from their IR and NMR spectra.

REFERENCE 9: 115:182703 Phenylacetylene dimerization promoted by ruthenium(II) complexes. Echavarren, Antonio M.; Lopez, Javier; Santos, Amelia; Montoya, Julio (Inst. Quim. Org., CSIC, Madrid, 28006, Spain).

J.

Organomet. Chem., 414(3), 393-400 (English) 1991. CODEN: JORCAI. ISSN: 0022-328X.

AB The complex $\text{Ru}(\text{CO})(\text{CH}:\text{CHPh})\text{Cl}(\text{C}_5\text{H}_5\text{N})(\text{PPh}_3)_2$ and related alkenyl complexes react in methanol or ethanol to give (E,E)-1,4-diphenylbuta-1,3-diene (I) and ruthenium(II) hydride $\text{Ru}(\text{CO})\text{H}(\text{Cl})(\text{C}_5\text{H}_5\text{N})(\text{PPh}_3)_3$. Further reaction of this hydride with the butadiene results in 1,2-redn. to yield (E)-1,4-diphenyl-1-butene. However, the reaction of phenylacetylene with catalytic amts. of ruthenium hydrides gave the dimer

(Z)-1,4-diphenylbuten-

3-yne. On the other hand, the reaction of 1,2-

diphenylethylenylruthenium(II) derivs. in methanol or ethanol gave

trans-stilbene rather than the butadiene. Several deuteration expts.

were

performed in order to elucidate the mechanism of formation of I and ruthenium hydride from the corresponding alkenyl complexes.

REFERENCE 10: 115:49952 The formation of alkenedithiocarboxylate and alkenecarboxylate ligands by insertion of carbon disulfide and dioxide into ruthenium(II)-alkenyl bonds. Loumrhari, Hassane; Ros, Josep; Yanez, Ramon; Torres, M. Rosario (Dep. Quim., Univ. Auton. Barcelona, Bellaterra,

08193, Spain). J. Organomet. Chem., 408(2), 233-9 (English) 1991.

CODEN:

JORCAI. ISSN: 0022-328X.

AB The unsatd. alkenyl complexes $\text{Ru}(\text{CO})\text{Cl}(\text{RC}:\text{CHR}')(\text{PPh}_3)_2$ react with CS_2 and CO_2 to give $\text{Ru}(\text{CO})\text{Cl}(\text{S}_2\text{CRC}:\text{CHR}')(\text{PPh}_3)_2$ and $\text{Ru}(\text{CO})\text{Cl}(\text{O}_2\text{CRC}:\text{CHR}')(\text{PPh}_3)_2$ complexes, resp. The products are hexacoordinated ruthenium(II)

complexes

contg. alkenedithiocarboxylate or alkenecarboxylate ligands

.eta.2-coordinated to metal. In these reactions CS_2 and CO_2 insert into ruthenium-alkenyl bonds to form new chelated ligands. The structures of products and the nature of the alkenedithiocarboxylate and alkenecarboxylate ligands were established from spectroscopic data (IR,

1H

and ^{31}P NMR).

L3 ANSWER 16 OF 19 REGISTRY COPYRIGHT 2001 ACS

RN 72068-25-8 REGISTRY

CN Dysprosium, diaquabis[4,4'-(1,2-ethenediyl)bis(pyridine)-N]tris(thiocyanato-N)-, homopolymer (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyridine, 4,4'-(1,2-ethenediyl)bis-, dysprosium complex, homopolymer

MF (C27 H24 Dy N7 O2 S3)x

CI PMS

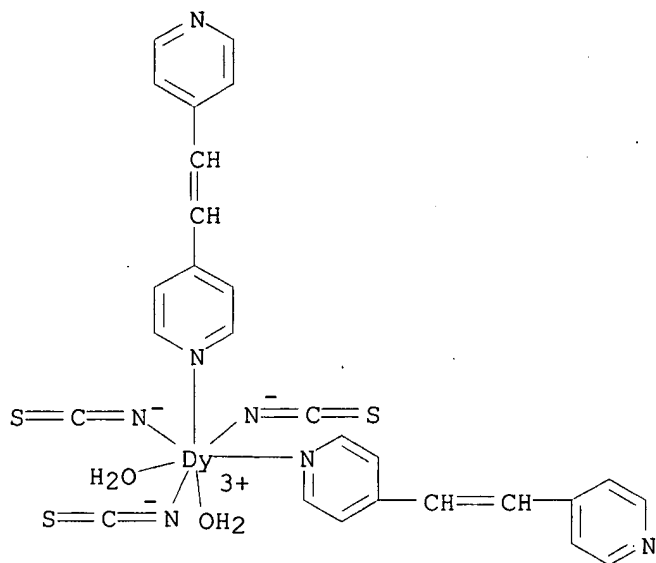
LC STN Files: CA, CAPLUS

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CRN 72068-24-7

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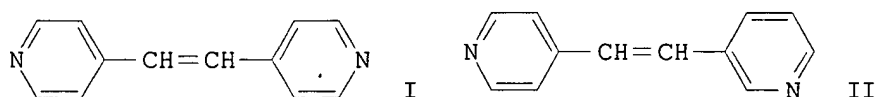
CCI CCS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 92:51136 Uranyl and lanthanide complexes of the 1,2-dipyridylethylene isomers. Seminara, A.; Giuffrida, S.; Bruno, G.; Siracusa, G.; Condorelli, G. (Ist. Chim. Gen., Univ. Catania, Catania, 8/95125, Italy). J. Inorg. Nucl. Chem., 41(5), 701-4 (English) 1979. CODEN: JINCAO. ISSN: 0022-1902.

GI

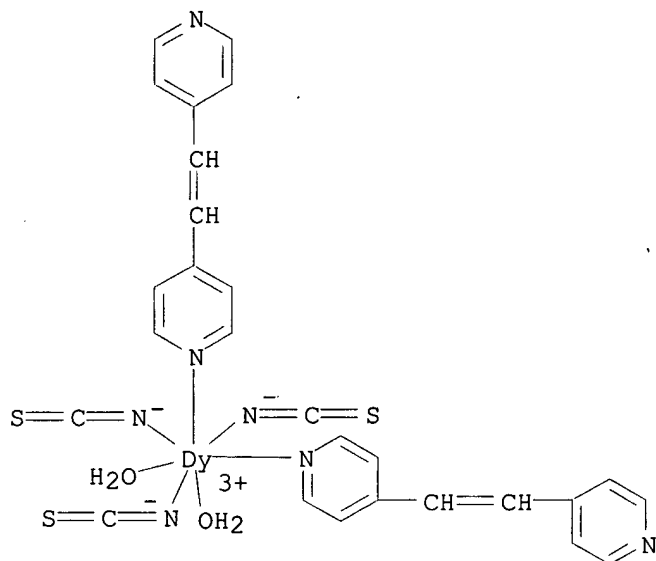


AB Uranyl and lanthanide complexes with the dipyridylethylene isomers I and II, e.g. $ML_2(NCS)_3$ ($M = La-Yb$; $L = I$), $UO_2L_1(OAc)_2$ ($L_1 = II$), were prepd. and characterized by elemental and thermal analyses, IR spectra, and cond.

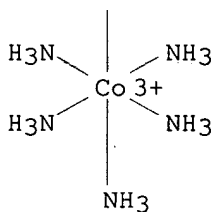
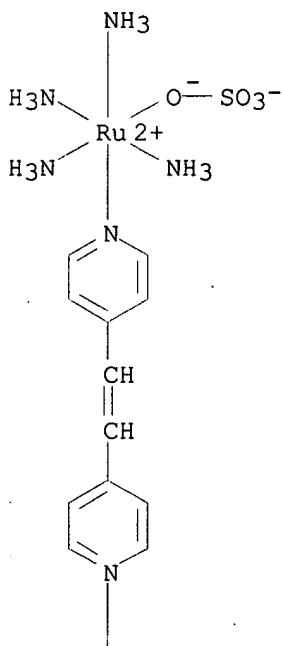
data. IR spectra showed that the diimine generally acts as a bidentate bridging ligand, although complexes with monodentate diimines were also formed. Enthalpy changes and activation energies for thermal decompn. of $ML_3(NO_3)_3$ ($M = La-Nd$, $Sm-Yb$) showed a periodic trend along the lanthanide series.

L3 ANSWER 17 OF 19 REGISTRY COPYRIGHT 2001 ACS
RN 72068-24-7 REGISTRY
CN Dysprosium, diaquabis[4,4'-(1,2-ethenediyl)bis(pyridine)]-

N]tris(thiocyanato-N)-(9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyridine, 4,4'-(1,2-ethenediyl)bis-, dysprosium complex
 MF C27 H24 Dy N7 O2 S3
 CI CCS, COM



L3 ANSWER 18 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 61158-47-2 REGISTRY
 CN Ruthenium(3+), tetraammine[.mu.-[4,4'-(1,2-ethenediyl)bis[pyridine]-N:N']](pentaamminecobalt)[sulfato(2-)-O]-, stereoisomer (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyridine, 4,4'-(1,2-ethenediyl)bis-, cobalt-ruthenium complex, (E)-
 CN Sulfuric acid, cobalt-ruthenium complex
 MF C12 H37 Co N11 O4 Ru S
 CI CCS
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

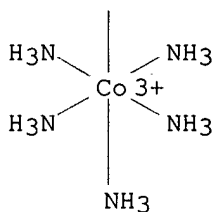
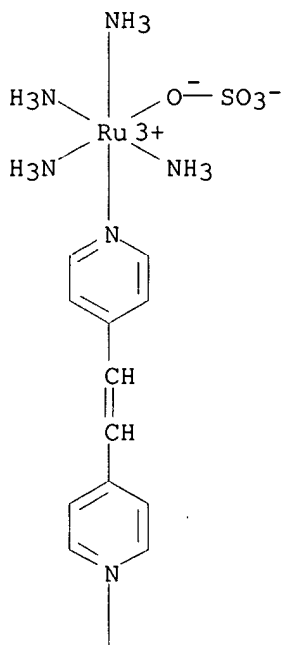
REFERENCE 1: 85:182867 Intramolecular electron transfer mediated by 4,4'-bipyridine and related bridging groups. Fischer, H.; Tom, G. M.; Taube, H. (Dep. Chem., Stanford Univ., Stanford, Calif., USA). J. Am. Chem. Soc., 98(18), 5512-17 (English) 1976. CODEN: JACSAT.

AB At 25.degree., the 1st-order specific rates for the redn. of Co(III) by Ru(II) in the complexes of the type [(NH3)5CoIIIL-LRuII(NH3)4H2O] with

L-L is 4,4'-bipyridine, 1,2-bis(4-pyridyl)ethylene, 3,3'-dimethyl-4,4'-bipyridine, bis(4-pyridyl) sulfide, and 1,2-bis(4-pyridyl)ethane are 44 .times. 10-3, 18.7 .times. 10-3, 5.5 .times. 10-3, 4.9 .times. 10-3, and

1.20 .times. 10⁻³ sec⁻¹, resp. The extinction coeffs. for the mixed valence species, [(NH₃(5RuIII-LRuII(NH₃)₅], with the same bridging ligands decrease in the same order as do the specific rates recorded, and a relation of at least limited validity between these 2 kinds of measurements is thereby indicated. For the Co(III)-Ru(II) complexes with the 1st 4 bridging ligands the values of activation enthalpy, .DELTA.H*, for intramol. electron transfer are within exptl. error const. (.DELTA.H* ranges from 20.0 to 20.3 kcal mole⁻¹) and the small differences in rate are reflected mainly in activation entropy, .DELTA.S*, which ranges from 2.6 cal degree⁻¹ mole⁻¹ for the fastest reaction to -1.9 for the slowest. These results suggest that the Franck-Condon barrier for electron transfer is const. for the series, and that the slight rate differences result from the slower reactions being not quite adiabatic. In the 4 systems referred to, the bridging group apparently mediates in electron transfer, but in the reaction with the bis(pyridyl)ethane ligand, electron transfer appears to take place directly between the metal centers.

L3 ANSWER 19 OF 19 REGISTRY COPYRIGHT 2001 ACS
 RN 60977-35-7 REGISTRY
 CN Ruthenium(4+), tetraammine[.mu.-[4,4'-(1,2-ethenediyl)bis[pyridine]-N:N']](pentaamminecobalt)[sulfato(2-)-O]-, tetrachloride, stereoisomer (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyridine, 4,4'-(1,2-ethenediyl)bis-, cobalt-ruthenium complex, (E)-
 MF C12 H37 Co N11 O4 Ru S . 4 Cl
 CI CCS
 LC STN Files: CA, CAPLUS



● 4. Cl⁻

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 85:182867 Intramolecular electron transfer mediated by 4,4'-bipyridine and related bridging groups. Fischer, H.; Tom, G. M.; Taube, H. (Dep. Chem., Stanford Univ., Stanford, Calif., USA). J. Am. Chem. Soc., 98(18), 5512-17 (English) 1976. CODEN: JACSAT.
AB At 25.degree., the 1st-order specific rates for the redn. of Co(III) by Ru(II) in the complexes of the type [(NH3)5CoIIIL-LRuII(NH3)4H2O] with L-L

is 4,4'-bipyridine, 1,2-bis(4-pyridyl)ethylene, 3,3'-dimethyl-4,4'-bipyridine, bis(4-pyridyl) sulfide, and 1,2-bis(4-pyridyl)ethane are 44×10^{-3} , 18.7×10^{-3} , 5.5×10^{-3} , 4.9×10^{-3} , and $1.20 \times 10^{-3} \text{ sec}^{-1}$, resp. The extinction coeffs. for the mixed valence species, $[(\text{NH}_3)_5\text{RuIII}(\text{L})\text{RuII}(\text{NH}_3)_5]$, with the same bridging ligands decrease in the same order as do the specific rates recorded, and a relation of at least limited validity between these 2 kinds of measurements is thereby indicated. For the Co(III)-Ru(II) complexes with the 1st 4 bridging ligands the values of activation enthalpy, ΔH^\ddagger , for intramol. electron transfer are within exptl. error const. (ΔH^\ddagger ranges from 20.0 to 20.3 kcal mole $^{-1}$) and the small differences in rate are reflected mainly in activation entropy, ΔS^\ddagger , which ranges from 2.6 cal degree $^{-1}$ mole $^{-1}$ for the fastest reaction to -1.9 for the slowest. These results suggest that the Franck-Condon barrier for electron transfer is const. for the series, and that the slight rate differences result from the slower reactions being not quite adiabatic. In the 4 systems referred to, the bridging group apparently mediates in electron transfer, but in the reaction with the bis(pyridyl)ethane ligand, electron transfer appears to take place directly between the metal centers.

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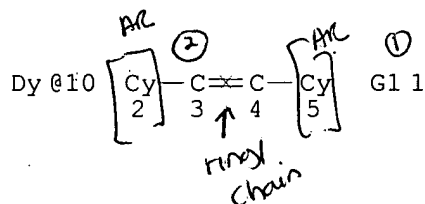
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L15 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2001 ACS

2001:64190 Document No. 134:126761 Multiplexed strand displacement method for nucleic acid sequence determinations using a combination of oligonucleotides. **Singh, Sharat**; Inamdar, Anita; **Ullman, Edwin F.**; Cao, Liching; Albagli, David (Aclara Biosciences, Inc., USA). PCT Int. Appl. WO 2001006008 A2 20010125, 49 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US18301 20000630. PRIORITY: US 1999-324629 19990716.

AB Multiplexed detns. of large nos. of events are achieved in an accurate and

simple manner by using a combination of different oligonucleotides, which serve for both capture and release from a support and strand displacement oligonucleotides for sequential release of groups of oligonucleotides. Also included, as part of the oligonucleotide reagents may be identifiers,

which serve to identify a particular characteristic. The method is illustrated using primers for initiation of chain extension joined to or serving as the capture/release sequence, where the extended primer has an identifier. After extending the primer, the extended primers are captured

and independently released and the released extended primers assayed. The

subject method finds application for nucleic acid sequence detns., single nucleotide polymorphism detns., identification of nucleic acid fragments, and the like.

L15 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2001 ACS

2000:814393 Sample evaporative control. **Singh, Sharat**; **Ullman, Edwin**; Gibbons, Ian; Boone, Travis; Xiao, Vivian; Bjornson, Torlief; Hooper, Herbert (Aclara Biosciences, Inc., USA). PCT Int. Appl. WO 2000067907 A2 20001116, 92 pp. DESIGNATED STATES: W: AE, AG, AL, AM,

AT,

AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US12826 20000510. PRIORITY: US 1999-PV133448 19990511; US 1999-PV140180 19990618; US 1999-470677 19991223.

AB Devices and methods are provided using microfluidic devices for manipulating small volumes and determining a variety of chemical and physical events. The devices rely upon an opening to the atmosphere of a small volume in a zone, where a sample is placed in the zone where

evaporation can occur. The zone is maintained in contact with a liquid medium that serves to replenish the liquid in the zone and maintain the composition of the mixture in the zone substantially constant. The diffusion of components in the zone is restricted during the course of the determination by the liquid flux into the zone.

L15 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2001 ACS
2000:688406 Document No. 133:248040 Methods for single nucleotide polymorphism (snp) detection. **Singh, Sharat; Ullman, Edwin F.** (Aclara Biosciences, Inc., USA). PCT Int. Appl. WO 2000056925 A2 20000928, 32 pp. DESIGNATED STATES: W: AU, CA, JP; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US6135 20000308. PRIORITY: US 1999-PV125319 19990319.

AB Methods and compns. are provided for detg. large nos. of single nucleotide polymorphisms in target DNA employing particles having (1) primers complementary to sequences in the target DNA where the next succeeding 3'-nucleotide is a potential single nucleotide polymorphism and coding compn. members, where the members are unique for each primer, and (2) differentially labeled terminating nucleotides, where the label permits sepn. of the terminating nucleotides. Desirably the particles are sepd. into groups having a common prevalent next succeeding nucleotide. The particles and target DNA are combined under nucleotide extending conditions, the particles sepd. into groups in accordance with the terminating nucleotide and the coding members identified, so that one knows the sequence and the single nucleotide polymorphism. Various protocols are provided for the detn.

L15 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2001 ACS
1999:549474 Document No. 131:167385 Chemiluminescent compositions for use in detection of multiple analytes. **Singh, Sharat; Ullman, Edwin F.** (Dade Behring Inc., USA). PCT Int. Appl. WO 9942838 A1 19990826, 71 pp. DESIGNATED STATES: W: AU, CA, JP; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US3207 19990215. PRIORITY: US 1998-25624 19980218.

AB Methods, compns. and kits are disclosed. The methods are directed to detg. the presence of relative amts. of two or more components in a medium. A combination is provided comprising a medium suspected of contg. the components and a label reagent for each of the components. The label reagent comprises a chemiluminescent compn. that is activated by electromagnetic radiation. A first specific binding pair (sbp) member may be assocd. with the reagent depending on the components to be detd. Luminescence emitted by each of the chemiluminescent compns. upon activation is differentially detectable. Where a first sbp member is employed, it is capable of binding to the component or to a second sbp member to form a complex related to the amt. of the component. At least one of the chemiluminescent compns. comprises a fluorescent energy acceptor. After the above are combined, the chemiluminescent compns. are activated. The amt. of luminescence generated by each of the

chemiluminescent compns. is detected and related to the amt. of each of the components in the medium.

L15 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2001 ACS

1997:740386 Document No. 128:11618 Chemiluminescent compositions and their use in the detection of hydrogen peroxide. **Ullman, Edwin F.; Singh, Sharat** (Behringwerke Aktiengesellschaft, Germany; Ullman, Edwin F.). PCT Int. Appl. WO 9741442 A1 19971106, 72 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US7265 19970501. PRIORITY: US 1996-17075 19960501.

AB Compns., methods, and kits are disclosed for detecting hydrogen peroxide or a compd. capable of generating hydrogen peroxide, esp. in clin. chem. The compns. comprise a matrix having incorporated therein a label capable of being modified by singlet oxygen. A catalyst capable of catalyzing

the

formation of singlet oxygen is bound to the matrix, which permits the diffusion of singlet oxygen therein. A sample suspected of contg. a compd. that can generate hydrogen peroxide is combined with a compn. in accordance with the present invention. The combination is subjected to conditions wherein such compd. generates hydrogen peroxide. The reaction of singlet oxygen with the label is detd., the reaction thereof

indicating

the presence of the compd. capable of generating hydrogen peroxide.

Examples are given of the detn. of glucose, cholesterol, theophylline, chorionic gonadotropin,.

L15 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2001 ACS

1997:15510 Document No. 126:44640 Metal chelate-containing compositions for use in chemiluminescent assays. **Singh, Sharat; Ullman, Edwin F.** (Behringwerke Ag, Germany). U.S. US 5578498 A 19961126, 23 pp. Cont.-in-part of U.S. Ser. No. 704,569. (English). CODEN: USXXAM. APPLICATION: US 1993-156181 19931122. PRIORITY: US 1991-704569 19910522.

AB Compns. are disclosed comprising (1) a metal chelate wherein the metal is selected from the group consisting of europium, terbium, dysprosium, samarium, osmium, and ruthenium in at least a hexa coordinated state and (2) a compd. having a double bond substituted with 2 aryl groups, an O atom, and an atom selected from the group consisting of O, S, and N, wherein one of the aryl groups is electron donating with respect to the other. Such compn. is preferably incorporated in a latex particulate material. Methods and kits are also disclosed for detg. an analyte,

e.g.,

T3, in a medium suspected of contg. the analyte. The methods and kits employ as one component a compn. as described above.

L15 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2001 ACS

1996:483856 Document No. 125:162775 Method and kits for determining peroxidatively active catalysts. **Singh, Sharat; Switchenko, Arthur C.; Lin, Cheng-I.; Kurn, Nurith; Ullman, Edwin F.** (Behringwerke Ag, Germany). U.S. US 5532138 A 19960702, 33 pp. Cont. of U.S. Ser. No. 951,922, abandoned. (English). CODEN: USXXAM. APPLICATION: US 1994-263164 19940621. PRIORITY: US 1990-516022 19900426; US 1992-951922 19920806.

AB Methods and compns. are disclosed for detg. a peroxidatively active catalyst, e.g., a peroxidase. The methods comprise the step of detecting

a substance formed by the coupling reaction of (1) the product of the peroxidatively active catalyst-catalyzed oxidn. of a benzidine with (2) a coupler other than benzidine. The methods have application in a wide variety of systems including assays for analytes, and esp. enzyme immunoassays. Also disclosed are kits for conducting methods and assays in accordance with the present invention, and examples are given for the detection of Chlamydia in a clin. sample taken on a swab and for the detection of HIV antibodies in blood.

L15 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2001 ACS

1996:316328 Document No. 125:1574 Luminescent oxygen channeling immunoassay (LOCI) for human thyroid stimulating hormone. **Ullman, Edwin F.**; Kirakossian, Hrair; **Singh, Sharat**; Irvin, Benjamin R.; Irvine, Jennifer D.; Wagner, Daniel B. (Research Department, Syva Company, Palo Alto, CA, 94303, USA). Biolumin. Chemilumin., Proc. Int. Symp., 8th, 16-19. Editor(s): Campbell, Andrew Keith; Kricka, Larry J.; Stanley, Philip E. Wiley: Chichester, UK. (English) 1994. CODEN: 62UZAR.

AB The authors describe an application of a new homogeneous chemiluminescent immunoassay procedure, luminescent oxygen channeling immunoassay (LOCI), and its application to assay of human TSH. The LOCI combines 2 prior concepts that have been used in homogeneous assays: latex agglutination

in

which an antibody, for example, can serve to aggregate latex particles that have been coated the corresponding antigen; and enzyme channeling immunoassay in which an immune reaction brings 2 enzymes into proximity near a surface, one of which catalyzes formation of a product that serves as a chromogenic substrate of the other enzyme. The method should permit detection of less than 60,000 TSH mols.

L15 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2001 ACS

1995:820770 Document No. 123:222300 Metal chelate containing compositions for use in chemiluminescent assays. **Ullman, Edwin F.**; **Singh, Sharat** (Syntex (U.S.A.) Inc., USA). PCT Int. Appl. WO 9514928 A1 19950601, 76 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1994-US13193 19941121. PRIORITY: US 1993-156181 19931122.

AB Compns. are disclosed comprising (a) a metal chelate wherein the metal is selected from the group consisting of europium, terbium, dysprosium, samarium, osmium and ruthenium in at least a hexacoordinated state and

(b)

a compd. having a double bond substituted with two aryl groups, an oxygen atom and an atom selected from the group consisting of oxygen, sulfur and nitrogen wherein one of the aryl groups is electron donating with respect to the other. Such compn. is preferably incorporated in a latex particulate material. Methods and kits are also disclosed for detg. an analyte in a medium suspected of contg. the analyte. The methods and

kits

employ as one component a compn. as described above.

L15 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2001 ACS

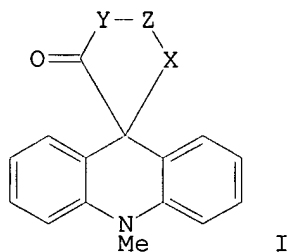
1994:477669 Document No. 121:77669 Luminescent oxygen channeling immunoassay: measurement of particle binding kinetics by chemiluminescence. **Ullman, Edwin F.**; Kirakossian, Hrair; **Singh, Sharat**; Wu, Z. Ping; Irvin, Benjamin R.; Pease, John S.;

Switchenko, Arthur C.; Irvine, Jennifer D.; Dafforn, Alan; et al. (Res. Dep., Palo Alto, CA, 94303, USA). Proc. Natl. Acad. Sci. U. S. A., 91(12), 5426-30 (English) 1994. CODEN: PNASA6. ISSN: 0027-8424.

AB A method for monitoring formation of latex particle pairs by chemiluminescence is described. Mol. oxygen is excited by a photosensitizer and an antenna dye that are dissolved in one of the particles. 1.DELTA.gO2 diffuses to the second particle and initiates a high quantum yield chemiluminescent reaction of an olefin that is dissolved in it. The efficiency of 1.DELTA.gO2 transfer between particles is .apprxeq.3.5%. The technique permits real-time measurement of particle binding kinetics. Second-order rate consts. increase with the no. of receptor binding sites on the particles and approach diffusion control. By using antibody-coated particles, a homogeneous immunoassay capable of detecting .apprxeq.4 amol of TSH in 12 min was demonstrated. Single mols. of analyte produce particle heterodimers that are detected even when no larger aggregates are formed.

L15 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2001 ACS
1994:212038 Document No. 120:212038 Chemiluminescent spiro-acridans, their preparation, and their use in analytical methodology. **Singh, Sharat**; Singh, Rajendra; Meneghini, Frank; **Ullman, Edwin F.** (Syntex (U.S.A.) Inc., USA). PCT Int. Appl. WO 9402486 A1 19940203, 50 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1993-US6636 19930719. PRIORITY: US 1992-916453 19920720.

GI



AB Spiro-acridans I [X, Y = O, S, Se, NH; Z = 1-5 atom chain; 0-8 H may be substituted by W (W = 1-50 non-H atoms); 1-4 of the arom. C may be replaced by N; 0-1 H may be substituted by org. radical] are disclosed, as are anal. methods using them. The anal. methods comprise e.g. (1) combining a medium suspected of contg. the analyte and a chemiluminescent compd., (2) combining a means for chem. activating the chemiluminescent compd.; and (3) detecting the amt. of luminescence generated by the chemiluminescent compd. The amt. of luminescence generated is related to the amt. of analyte in the medium. The chemiluminescent compd. can be chem. activated by hydrogen peroxide. Compns. and kits are also disclosed. Prepn. of selected I is described. Thus, II, prepd. from

10-methylacridinium-9-carboxylate and 1,2,4-trihydroxybenzene, showed enhanced chemiluminescence with horseradish peroxidase.

=> s l11 and metal chelat?

1211546 METAL

590921 METALS

1451134 METAL

(METAL OR METALS)

102486 CHELAT?

11488 METAL CHELAT?

(METAL(W)CHELAT?)

L16 0 L11 AND METAL CHELAT?

=> s l11 and ?assay?

430750 ?ASSAY?

L17 0 L11 AND ?ASSAY?

=> fil reg

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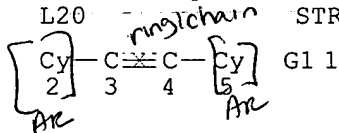
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
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21 ANSWERS

L22 2 L21 NOT L3

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L22 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2001 ACS

RN 62828-46-0 REGISTRY

CN Ruthenium,

octacarbonylbis(1-methyl-2,3,4,5-tetraphenylsilacyclopenta-2,4-
dien-1-yl)di-, (Ru-Ru) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

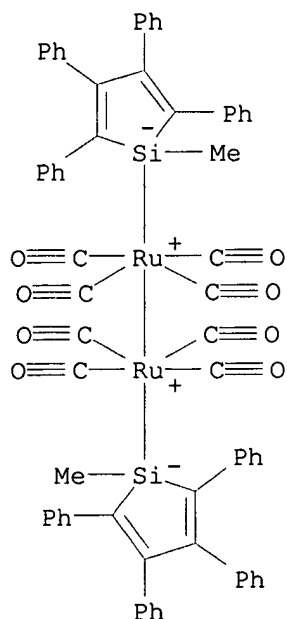
CN Silacyclopenta-1,4-diene, 1-methyl-2,3,4,5-tetraphenyl-, ruthenium
complex

CN Silacyclopentane, ruthenium deriv.

MF C66 H46 O8 Ru2 Si2

CI CCS

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:171551 Silacyclopentadiene complexes of molybdenum, chromium, iron, ruthenium, cobalt, and rhodium. Abel, Edward W.; Blackmore, Timothy; Whitley, Robert J. (Dep. Chem., Univ. Exeter, Exeter, Engl.). J. Chem. Soc., Dalton Trans. (23), 2484-9 (English) 1976.

CODEN:

JCDTBI.

GI For diagram(s), see printed CA Issue.

AB Transition metal complexes of 3 substituted silacyclopentadienes were prepd. and different stoichiometries and modes of bonding were obsd. Mo(CO)₆ formed the bis(diene) complex MoL₂(CO)₂ (L = I) but with Cr(CO)₆ the arene complex II was formed. A CO-bridged complex Co₂L₂(CO)₄ was isolated from the Co₂(CO)₈ reaction but a hexacarbonyl complex formed could not be isolated. (RhCl)₂ and [Rh(CO)₂Cl]₂L were prepd. from [Rh(CO)₂Cl]₂, the former having a Cl bridge and the latter a bridging silacyclopentadiene group. The substituted silacyclopentadiene III with Fe₃(CO)₁₂ gave the endo-H form of FeL(CO)₃ (L = III) and with Ru₃(CO)₁₂ gave IV contg. a Si-Ru-Ru-Si sequence. I and the substituted silacyclopentadiene V with Ru₃(CO)₁₂ gave RuL(CO)₃ (L = I, V, resp.). Structural and spectroscopic characteristics of the complexes were detd. and compared with related species.

L22 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2001 ACS

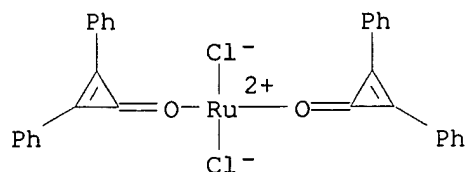
RN 16092-11-8 REGISTRY

CN Ruthenium, dichlorobis(diphenylcyclopropenone)-, trans- (8CI) (CA INDEX NAME)

MF C30 H20 Cl2 O2 Ru

CI CCS

LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 67:82252 Organometallic intermediates. II. Preparation and structure of some diphenylcyclopropenone complexes. Bird, Clive W.; Briggs, Elizabeth M. (Queen Elizabeth Coll. London, London, Engl.). J. Chem. Soc. A (7), 1004 (English) 1967. CODEN: JCSIAP.
AB cf. CA 67: 63472j. A series of complexes of diphenylcyclopropenone with zinc(II), cobalt(II), nickel(II), copper(II), ruthenium(II), rhodium(III), palladium(II), and platinum (IV) and -(II) were prepd. The structures of these complexes elucidated by spectroscopic and magnetic measurements, and the position of diphenylcyclopropenone in the spectrochem. series detd. In all cases coordination occurs through the carbonyl O.

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